

Line Shape of the $\mu\text{H}(3p - 1s)$ Hyperfine Transitions

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The $(3p - 1s)$ x-ray transition to the muonic hydrogen ground state was measured with a high-resolution crystal spectrometer. A Doppler effect broadening of the x-ray line was established which could be attributed to different Coulomb deexcitation steps preceding the measured transition. The assumption of a statistical population of the hyperfine levels of the muonic hydrogen ground state was directly confirmed by the experiment, and measured values for the hyperfine splitting can be reported. The results allow a decisive test of advanced cascade model calculations and establish a method to extract fundamental strong-interaction parameters from pionic hydrogen experiments.

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A series of experiments has been conducted at the Paul Scherrer Institut (PSI), Switzerland, to extract the isospin separated pion-nucleon scattering lengths from the observation of x-ray transitions feeding the ground state of pionic hydrogen [1–3]. With x-ray energies of about 2–3 keV and values for the strong-interaction shift and broadening being of about 7 and 1 eV, respectively, the use of a high-resolution Bragg spectrometer was mandatory to reach the envisaged precision on the percent level.

The experimental difficulties are considerable, especially for the isovector scattering length, which is equivalent to the determination of the strong interaction broadening. It imposes the requirement to extract from the measured line shape a Lorentzian profile representing the natural width, which is convoluted with the spectrometer response and several contributions owing to the Doppler broadenings from different high velocity states of the exotic atom.

High velocity states develop in exotic hydrogen atoms during the atomic deexcitation cascade. As the system is electrically neutral, it may dive deeply into the electron cloud of a neighboring hydrogen molecule. Such close collisions strongly influence the atomic cascade. The most important of these processes are the so-called Coulomb transitions [4–6], collision-induced radiationless deexcitations, where the released energy is shared between the exotic atom and a normal hydrogen atom as recoil partner. During the cascade, acceleration due to Coulomb transitions and deceleration by elastic and inelastic collisions compete, which results in a complex and level dependent kinetic energy distribution.

Historically, the first evidence for high velocity states was found in the charge exchange reaction $\pi^- p \rightarrow \pi^0 n$ with stopped pions as Doppler broadening of the time-of-flight (TOF) of the monoenergetic neutrons [7]. Later on, detailed studies confirmed that Coulomb deexcitation substantially affects the kinetic energy of πH [8] and μH atoms [9] even at lowest densities. From the TOF spectra, several components were identified and attributed to specific Coulomb transitions. Hints for the influence of the Doppler broadening in x-ray transitions were identified in experiments measuring the strong-interaction width of the πH ground state [2,3]. A correction for the cascade-induced broadening is therefore indispensable for a proper extraction of the hadronic contribution to the x-ray line-width. However, the high precision information from the reaction $\pi^- p \rightarrow \pi^0 n$ cannot be directly transferred to x-ray studies. Charge exchange occurs from ns states, mainly with principal quantum numbers $n = 3$ –5 of the $\pi^- p$ system, whereas the initial states for K x-ray emission are np levels. Consequently, the preceding cascade steps for the two processes are different, and the Doppler contributions to the x-ray line shape deviate from the ones derived from neutron TOF experiments.

As the intensities of the x-ray transitions strongly depend on the hydrogen density, there was a first approach to extract information about the cross sections of Coulomb deexcitation from intensity studies. Different processes such as Stark transitions and external Auger effect, however, are overwhelming in their importance for the x-ray intensity compared to Coulomb deexcitation. In consequence, the kinetic energy T_{kin} of the exotic hydrogen

atom was used in earlier cascade codes (the so-called Standard Cascade Model: SCM) as a fitting parameter with values around $T_{\text{kin}} = 1$ eV, which explained the measured intensities with sufficient accuracy [10].

Based on the SCM, an extended standard cascade model (ESCM) was developed. It is a new approach to calculate the Doppler contributions to neutron TOF and exotic hydrogen x-ray spectra by taking into account the competing processes in each deexcitation step and, hence, is able to provide the kinetic energy distribution at the time of x-ray emission [11]. An example of such a kinetic energy distribution for muonic hydrogen in the $3p$ state is shown in Fig. 1. Monoenergetic lines corresponding to specific Coulomb transitions $n \rightarrow n'$ are smeared out because of the numerous elastic collisions after the Coulomb transition and before x-ray emission. The validity of ESCM calculations cannot be tested directly in pionic hydrogen as the strong-interaction broadening completely masks the fine details of the various Doppler contributions.

Muonic hydrogen as a purely electromagnetic twin system to pionic hydrogen offers itself as an ideal candidate for the direct observation of the Coulomb deexcitation. Ideally, it could be used as a test of the validity of the ESCM by reproducing the line shape of muonic hydrogen x-ray transitions in a fitting routine with the predictions of the ESCM as input. The theoretical values for the ground-state hyperfine splitting, and more important, for the relative intensity of the transitions feeding the triplet and singlet components, should be obtained. The ground-state hyperfine splitting is calculated to be 182.725 ± 0.062 meV [12]. A relative statistical population of 3:1 is expected for the triplet and singlet components.

An understanding of the atomic cascade in exotic hydrogen is needed in other experimental studies as well, e.g., (i) for the precision determination of the proton charge

radius from the muonic hydrogen $2s - 2p$ Lamb shift [9,13] or (ii) in the measurement of the induced pseudo-scalar coupling in muon capture by the proton [14–16].

The experiment was performed at the $\pi E5$ channel of the proton accelerator at PSI, which provides a low-energy pion beam with intensities of up to a few $10^8/\text{s}$. Pions of 112 MeV/ c were injected into the cyclotron trap II [1] and decelerated using a set of degraders optimized to the number of muon stops by measuring x-rays from muonic helium. Muonic atoms are formed by slow muons originating from the decay of almost stopped pions close to or in a cylindrical cryogenic target cell of 22 cm length and 5 cm in diameter in the center of the trap. The cell was filled with hydrogen gas cooled down to 25 K at 1 bar absolute pressure, which corresponds to a density equivalent to 12.5 bar at room temperature. X radiation could exit the target cell axially through a 5 μm thick Mylar® window.

X rays from the $\mu\text{H}(3p - 1s)$ transition were measured with a Johann-type Bragg spectrometer equipped with a spherically bent Si(111) crystal having a radius of curvature of 2982.2 ± 0.3 mm and a free diameter of 90 mm [17]. Such a spectrometer is able to measure simultaneously an energy interval according to the width of the x-ray source when using a correspondingly extended x-ray detector, in this case a 3×2 array of charge-coupled devices (CCDs) covering in total 72 mm in height and 48 mm in width [18]. A pixel size of 40 μm provides the two dimensional position resolution necessary in order to measure the diffraction image. The background rejection capability of CCDs together with a massive concrete shielding suppresses efficiently events from beam induced reactions. In total, almost 10 000 events were collected for the $\mu\text{H}(3p - 1s)$ line (Fig. 2).

The spin-averaged $\mu\text{H}(3p - 1s)$ transition energy is calculated to be 2249.461 ± 0.001 eV with a radiative linewidth of 0.3 μeV [19]. The $3p$ -level splittings amount to a few meV only [20]. Hence, two components with identical response functions are sufficient to describe the $(3p - 1s)$ line. The spectrometer response was determined using narrow x-rays from helium-like argon as outlined in [21,22]. Applying this method to chlorine and sulfur, an extrapolation yields a resolution of 272 ± 3 meV (FWHM) at the $\mu\text{H}(3p - 1s)$ transition energy, which is significantly narrower than the observed linewidth (Fig. 2). Details may be found elsewhere [23].

As a first trial to include the Doppler broadening caused by Coulomb deexcitation, the kinetic energy distribution given by the ESCM result of [11] (Fig. 1) was taken directly as an input for the fitting of the line shape, which was done by means of the MINUIT package [24]. A comparison to the measured line shape yields a poor reduced χ^2 of $\chi^2_r = 1.353$ only (Fig. 2, dashed-dotted line).

It is evident that this ESCM prediction with a weight of 36% only for the low-energy component $T_{\text{kin}} \leq 2$ eV underestimates substantially the fraction of x-rays with

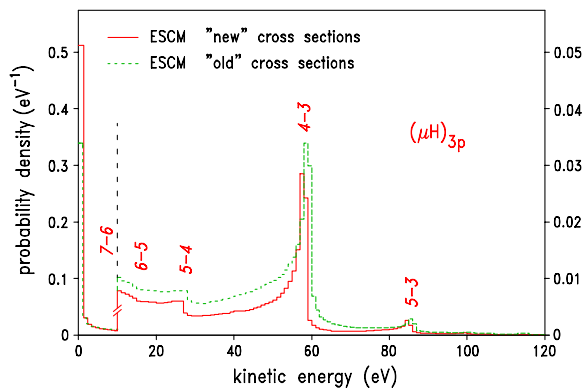


FIG. 1 (color online). Kinetic energy distribution of μH atoms in the $3p$ state for a hydrogen density equivalent to 12.5 bar as predicted from the ESCM [11] using cross sections calculated by [11] (dashed curve) and recalculated cross sections [26] stimulated by the present experiment (solid curve). Numbers indicate the corresponding Coulomb transitions $n \rightarrow n'$. Note the change of the vertical scale at 10 eV.

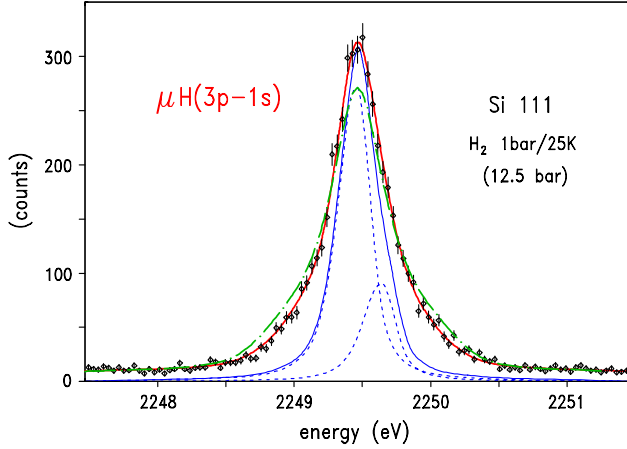


FIG. 2 (color online). Line shape of the $\mu\text{H}(3p-1s)$ transition as measured with a Si (111) crystal in first order. One energy bin corresponds to 2 CCD pixels or 37.2 meV. The spectrometer response (thin solid line) represents the expected line shape formed by the two hyperfine components (dashed lines) without any Doppler broadening (normalized to the peak height after background subtraction). Including Coulomb deexcitation by using longstanding cross sections [11] yields a poor description (dashed-dotted) of the line shape. The “best fit” in a “model free” approach (see text) is shown by thick solid line following the data. A very good fit—being indistinguishable by eye from the “model free” approach—was found when using for the ESCM calculation the recently recalculated cross sections [26].

small Doppler shifts. This reveals that cross sections responsible for the development of such low energies coming from an interplay of Coulomb deexcitation and elastic collisions could still be deficient. In addition, the cascade calculation starting at $n = 8$ possibly neglects stronger effects from Coulomb deexcitation in the outer shells ($n > 11$), where the ESCM uses a classical trajectory Monte Carlo approach.

Consequently, as a further approach, a “model free” method was applied, which has already been used in the case of the neutron TOF spectra [8]. The Doppler contributions from Coulomb deexcitation to the $\mu\text{H}(3p-1s)$ line shape were determined by modelling the kinetic energy distribution with several rectangular boxes, the number of which is assessed by the transitions in the preceding cascade.

Several sets of kinetic energy boxes were investigated including besides $\Delta n = 1$ also $\Delta n = 2$ Coulomb transitions. Hyperfine splitting, i.e., both line positions, relative population, (flat) background, and the relative weight of the boxes were free parameters in the fit. The sum of the relative weights of the boxes was always normalized to one.

It is a major result of this study that three narrow boxes are essential but also sufficient to model a kinetic energy distribution yielding a good fit to the $\mu\text{H}(3p-1s)$ line shape: (i) one low-energy component below $T_{\text{kin}} = 2$ eV collecting μH atoms which gained their energy from $n \geq$

10 Coulomb transitions and/or high velocity systems degraded by collisions, and (ii) two at higher energies corresponding to the deexcitation steps $n = 5 \rightarrow 4$ ($T_{\text{kin}} = 26.9$ eV) and $n = 4 \rightarrow 3$ ($T_{\text{kin}} = 58.2$ eV).

A χ^2 analysis shows that a weight of $\approx 60\%$ is mandatory for the low-energy component. In case of the high-energy components, the fit is only sensitive to the relative weight and the central value. Extending the boundaries up to $\pm 30\%$ of the central values affects the result by less than 1.4 standard deviations. Therefore, the kinetic energy distribution could be condensed to three narrow intervals.

The best reduced χ^2 is found to be $\chi_r^2 = 0.947$ for the kinetic energy intervals set to $[0-1.8]$, $[26.4-27.4]$, and $[57.7-58.7]$ eV resulting in relative weights of $(61 \pm 2)\%$, $(25 \pm 3)\%$, and $(14 \pm 4)\%$ (Fig. 2: “best fit” in the “model free” approach). Uncertainties represent statistical errors only.

A correlation study of hyperfine splitting and relative population was performed by using the three kinetic energy intervals found in the above mentioned analysis, but with their weights, total intensity, and background kept as free parameters. The best $\chi_r^2 = 0.941$ is obtained for a hyperfine splitting of 211 ± 19 meV, a triplet-to-singlet population of $(3.59 \pm 0.51) : 1$ (Fig. 3, A), and relative weight of $61 \pm 1\%$ for the low-energy component, where errors correspond to 1σ . The 1, 1.5, and 2σ contours are also shown. When fixing the hyperfine splitting to the theoretical value, the best fit is obtained for a triplet-to-singlet population of $(2.90 \pm 0.21) : 1$ (Fig. 3, B), very close to the statistical value. The χ^2 differs only by 1.5σ from the best value.

The results from the present experiment led to a reconsideration of cross sections involved in exotic-hydrogen deexcitation. In a fully quantum-mechanical close-coupling approach, elastic scattering, Stark transitions, and Coulomb deexcitation now have been calculated in a unified manner [5,6,25].

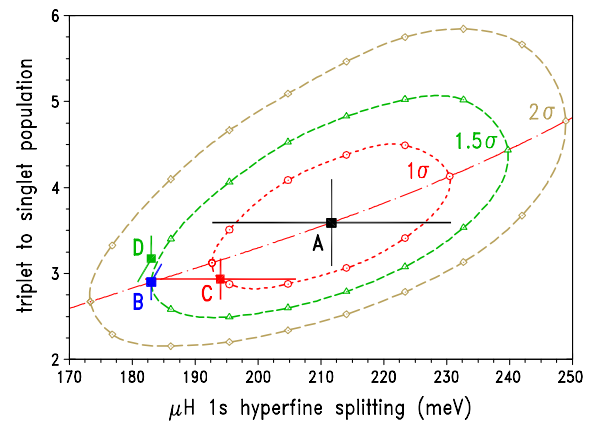


FIG. 3 (color online). χ^2 contour for the correlation of hyperfine splitting and relative population in the “model free” approach. The dashed-dotted line displays the location of the minimum χ^2 for the corresponding hyperfine splitting. (A–D: see text).

Including these cross-section results in the ESCM model [26], the relative weight of the low energies ($T_{\text{kin}} \leq 2$ eV) increases to 55%, which is closer to the constraint found in the “model free” approach. A fit to the measured $\mu\text{H}(3p - 1s)$ line shape by using directly the new kinetic energy distribution (Fig. 1) yields a much better description of the data (Fig. 2). Leaving hyperfine splitting and triplet-to-singlet intensity ratio as free parameters, values were obtained of 194 ± 12 meV for the hyperfine splitting and $(2.94 \pm 0.24) : 1$ for the triplet-to-singlet intensity ratio (Fig. 3, C). The striking agreement is indicated by $\chi_r^2 = 0.997$. When fixing the splitting to the theoretical value, the relative triplet-to-singlet population becomes $(3.17 \pm 0.27) : 1$ (Fig. 3, D).

Another process, which may affect the line shape, is due to molecule formation with subsequent radiative decay $(\mu p)_{\text{nl}} + \text{H}_2 \rightarrow [(\mu pp)^* \text{pee}]^* \rightarrow [(\mu pp) \text{pee}]^* + \gamma$ [27,28]. If radiative decay contributes significantly, a line broadening or even satellites at the low-energy side are expected. In the case of μpp , a branching ratio for radiative decay was predicted at the few per cent level [29,30]. However, in this experiment, no evidence was found at the 1% level for any broadening except from Coulomb deexcitation. The result is corroborated from the absence of any density dependence of the $\pi\text{H}(3p - 1s)$ transition energy [3].

To summarize, the line shape of the $\mu\text{H}(3p - 1s)$ transition was measured with a high-resolution Bragg spectrometer. The influence of Coulomb deexcitation was directly seen from a line broadening compared to the spectrometer resolution. By using a “model free” approach, various Doppler contributions are identified, which are attributed to preceding Coulomb transitions. A large fraction of the μH systems are found to have kinetic energies below 2 eV. The measurement yields the μH ground-state hyperfine splitting as calculated from QED and confirms experimentally the statistical population of the triplet and singlet $1s$ states. The measurement triggered a new calculation of cross sections resulting in a significantly improved description of the $\mu\text{H}(3p - 1s)$ line shape and serves as a basis for a further evaluation of the determination of the isovector scattering amplitude from pionic hydrogen data with increased precision.

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